Nucl. Sci. and Tech., Vol.8, No. 4 (2018), pp. 10-19

Nuclear Science and Technology

Journal homepage: https://jnst.vn/index.php/nst

Burnup calculation of the OECD VVER-1000 LEU benchmark assembly using MCNP6 and SRAC2006

Nguyen Huu Tiep*, Nguyen Thi Dung, Tran Viet Phu, Tran Vinh Thanh and Pham Nhu Viet Ha

Institute for Nuclear Science and Technology, Vietnam Atomic Energy Institute
179 Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam
**Email: tiepngh@gmail.com*

Abstract: The present work aims to perform burnup calculation of the OECD VVER-1000 LEU (low enriched uranium) computational benchmark assembly using the Monte Carlo code MCNP6 and the deterministic code SRAC2006. The new depletion capability of MCNP6 was applied in the burnup calculation of the VVER-1000 LEU benchmark assembly. The OTF (on-the-fly) methodology of MCNP6, which involves high precision fitting of Doppler broadened cross sections over a wide temperature range, was utilized to handle temperature variation for heavy isotopes. The collision probability method based PIJ module of SRAC2006 was also used in this burnup calculation. The reactivity of the fuel assembly, the isotopic concentrations and the shielding effect due to the presence of the gadolinium isotopes were determined with burnup using MCNP6 and SRAC2006 in comparison with the available published benchmark data. This study is therefore expected to reveal the capabilities of MCNP6 and SRAC2006 in burnup calculation of VVER-1000 fuel assemblies.

Keywords: *VVER-1000 LEU fuel assembly, fuel burnup, MCNP6, SRAC2006.*

I. INTRODUCTION

The United States and Russian Federation, under a mutual agreement, have been working towards the final disposition of weapons-grade (WG) surplus plutonium in each country as mixed-oxide (MOX) fuel in existing commercial nuclear reactors. To support this mission, the OECD/NEA established an international Experts Group to facilitate the sharing of existing information and experience and to deal with the physics and fuel behavior of MOX fuel as it relates to the WG plutonium disposition. Recent work in Russia, where WG MOX fuel will be used in both fast reactor (BN-600) and light water reactors (VVER-1000), has focused on the certification of the calculation codes and the design of MOX fuel assemblies and core configurations. In this regard, the Experts Group has carried out a benchmarking effort called the OECD VVER-1000 LEU (low enriched uranium) and MOX assembly computational benchmark for verification of the Russian calculation codes and methods in support for the WG plutonium disposition mission [1]. The benchmark consists of two different hexagonal fuel assemblies: a uniform LEU fuel assembly with 12 UGD (uranium-gadolinium) rods and a profiled MOX fuel assembly with 12 UGD rods. These two assemblies are representative of the advanced

https://doi.org/10.53747/jnst.v8i4.62
Received 16 November 2018, accepted 28 November 2018

designs under active R&D in Russia for VVER-1000 reactors and similar to the designs that are expected to be used in the plutonium disposition mission. Various solutions of the benchmark are reported in the literature and they are based on different calculation codes and nuclear data libraries [1-7]. Most of these solutions have been obtained by means of collision probability or similar methodologies, while few of them are based on Monte Carlo methods.

In Vietnam, the reactor fuel management in general and fuel burnup calculation in particular have been studied for years, especially for the Dalat Nuclear Research Reactor (DNRR) [8-10]. While a huge experience with the fuel burnup calculation of the DNRR has been accumulated over 30 years, there are only few publications related to fuel burnup calculation for power reactors like VVER-1000. In 2016, Hiep et al. [11] developed an MCNP5-ORIGEN coupling scheme for burnup calculation of VVER-1000 fuel assemblies. The coupling scheme was verified against the OECD VVER-1000 LEU benchmark assembly [1]. However, the predictor-corrector method has not yet been applied in the scheme and this can result in potential errors during the burnup calculation. Additionally, only the cross sections for 24 actinides and 61 fission products were used in this verification due to the unavailability of many MCNP5 cross sections.

The present work aims at performing a comparative burnup analysis of the OECD VVER-1000 LEU computational benchmark assembly using the Monte Carlo code MCNP6 [12] and the deterministic code SRAC2006 [13]. The new depletion capability of MCNP6 will be applied in the burnup calculation for the VVER-1000 LEU assembly. The On-The-Fly (OTF) methodology for MCNP, which involves high precision fitting of Doppler broadened cross sections over a wide temperature range, will be utilized to handle temperature variation for heavy isotopes [14]. In addition, the collision probability method based PIJ module of SRAC2006 will also be utilized in the burnup calculation of the VVER-1000 LEU assembly. The ENDF/B-VII.0 nuclear data library will be used in the MCNP6 and SRAC2006 calculations, respectively. This study is therefore expected to reveal the capabilities of MCNP6 and SRAC2006 in burnup calculation of VVER-1000 fuel assemblies.

II. CALCULATION METHODOLOGY

The VVER-1000 LEU benchmark hexagonal assembly consists of 300 fuel pin cells with 3.7 wt% ^{235}U, 12 UGD (Uranium-Gadolinium) pin cells with 3.6 wt% ^{235}U and 4 wt% Gd_2O_3, 18 water filled guide tubes for control rod insertion and one central water filled instrumentation tube. The configuration and main design parameters of the VVER-1000 LEU fuel assembly are shown in Fig. 1 and Table I, respectively. Detailed information of material composition and geometry of fuel pins, cladding, moderator, UGD pins, central and guide tubes, etc. can be easily found in Ref. [1]. The cell numeration of the one-sixth of the fuel assembly for simulating different isotopic compositions is illustrated in Fig. 2.

The burnup calculation for the VVER-1000 LEU benchmark assembly under the hot operating poisoned condition (the S1 state) will be performed using MCNP6 and SRAC2006. Under this condition, the fuel temperature is 1027 K and the moderator temperature is 575 K with equilibrium ^{135}Xe and ^{149}Sm concentrations and a power density of 108 MWt/m^3 up to a burnup 40 MWd/kgHM. In the MCNP6 and SRAC calculations, the UGD rods are divided into 5 annuli of equal area as required in the benchmark document [1] in order to account for the shielding effect due to the gadolinium isotopes. This allows the calculation of nuclide concentrations as a function of the radial position in the UGD rods.

In the MCNP6 simulation, the statistical error of ~30 pcm was obtained as the neutron history of $5x10^6$ for parallel depletion calculation was selected and the burnup calculation was performed with 160 steps of 0.25 MWd/kgHM. MCNP6 includes the new depletion capability that links steady state flux calculations in MCNP6 and nuclide depletion calculations in CINDER90. A steady state flux calculation is run in MCNP6 to determine the system eigenvalue, group fluxes, energy integrated reaction rates, fission multiplicity, and recoverable energy per fission. CINDER90 then uses these values generated by MCNP6 to perform depletion calculation to generate new number densities for the next time step. MCNP6 takes the new number densities generated by CINDER90 for the next steady state flux calculation. This linked process is repeated until the end of the final time step. It is noted that CINDER90 contains transmutation data information for over 3400 isotopes, 1325 fission products, yield set for 30 actinides.

However, the default nuclear data in MCNP6 are given at certain temperatures for heavy isotopes (293.6, 600, 900, 1200 and 2500K); while the fuel temperature of 1027K is needed in this calculation. There are various methods to cope with such kind of temperature dependence [14]. One of the suitable methods for MCNP6 is the OTF methodology for fitting of Doppler broadened cross sections and this method was applied in this study. The OTF data for heavy isotopes in the VVER-1000 LEU benchmark assembly that correspond to the temperature range of 293.6 to 1200 K were created from the ENDF/B-VII.0 library at the temperature of 293.6 K.

The PIJ module with its cell burnup routine of the SRAC2006 code system was also utilized for the burnup calculation of the VVER-1000 LEU benchmark assembly. The PIJ module that is based on the collision probability method was used for lattice cell calculations. The cell burnup routine used one-group collapsed flux distribution and the collapsed microscopic cross sections to solve the depletion equation using the Bateman's method. The burnup calculation using the cell burnup routine of the PIJ module was performed with 40 steps of 0.25 MWd/kgHM followed by 5 steps of 1.0 MWd/kgHM and 10 steps of 2.5 MWd/kgHM. The 107 neutron energy groups based on the ENDF/B-VII.0 library were collapsed to four groups for use in the SRAC2006 calculations.

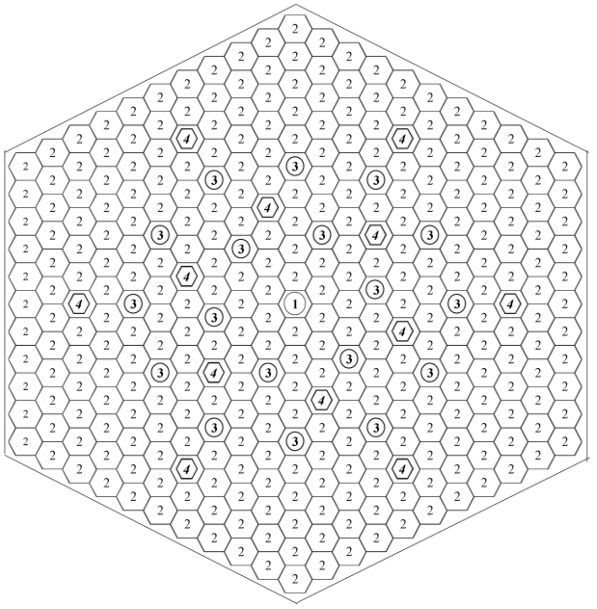

Fig. 1. VVER-1000 LEU benchmark assembly configuration

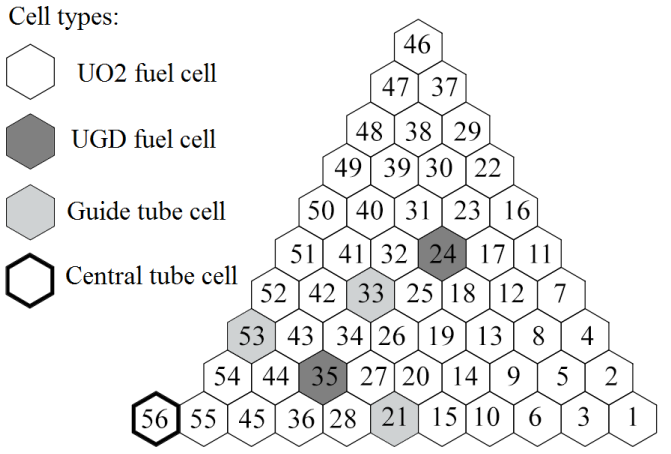

Fig. 2. Cell numeration in the one-sixth of VVER-1000 LEU benchmark assembly

Table I. Main design parameters of VVER-1000 LEU benchmark assembly

Parameter	Value
Number of UO_2 fuel cells	300
Number of fuel cells with Gd	12
Number of guide tubes	18
Number of central tubes	1
Fuel cell inner radius, cm	0.3860
Fuel cell outer radius, cm	0.4582

Central tube cell inner radius, cm	0.5450
Central tube cell outer radius, cm	0.6323
Pin pitch, cm	1.2750
Fuel assembly pitch, cm	23.6
^{235}U enrichment, wt%	3.7
Gd_2O_3 density, g/cm^3	7.4

III. RESULTS AND DISCUSSION

A. Infinite multiplication factor versus burnup

The infinite multiplication factor (k-inf) of the VVER-1000 LEU benchmark assembly as a function of burnup was calculated using MCNP6 and SRAC2006. It was found that the k-inf results obtained with MCNP6 and SRAC2006 compare well with the benchmark mean (BM) values as shown in Fig. 3. The k-inf values calculated with MCNP6 and SRAC2006 were slightly different from the BM values at the first burnup steps and such difference became significantly bigger after about 5 MWd/kgHM. After the gadolinium burns out, the k-inf value calculated by SRAC2006 and the BM value tend to approach to each other and their differences with that calculated by MCNP6 become roughly stable. The maximum differences in the k-inf calculated with MCNP6 and SRAC2006 with the BM values are 413 pcm and 352 pcm, respectively; whereas those for MCU, TVS-M, WIMS8A, HELIOS, MULTICELL [1], and MCNP5-ORIGEN [11] are 440, 400, 460, 260, 360, and 585 pcm, respectively.

As can be seen in Fig. 3, the reactivity of the fuel assembly slightly increases with burnup at the beginning of the cycle thanks to the use of Gd_2O_3 in the UGD pins for excess reactivity control. As the gadolinium isotopes burn out, the reactivity starts to decrease with burnup in a nearly linear manner due to the effect of fissile material depletion and neutron absorber accumulation. It was also seen that the effect on reactivity of the gadolinium burnable absorber and the time at which the reactivity starts to decrease can be well simulated by MCNP6 and SRAC2006.

B. Concentration of isotopes versus burnup

The variation of the concentration of the nuclides ^{235}U, ^{236}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{135}Xe, ^{149}Sm, ^{155}Gd, ^{157}Gd in Cell 1 and Cell 24 (see Fig. 2) as a function of burnup was calculated using MCNP6 and SRAC2006 in comparison with the BM values as shown in Figs. 4 and 5. It can be seen that the isotopic concentrations calculated by MCNP6 and SRAC2006 generally agree well with the BM values. The maximum deviations of the MCNP6 and SRAC2006 results with the BM values for Cell 1 are -7.93% for ^{149}Sm and 7.29% for ^{239}Pu at the end of the burnup (40 MWd/kgHM), respectively.

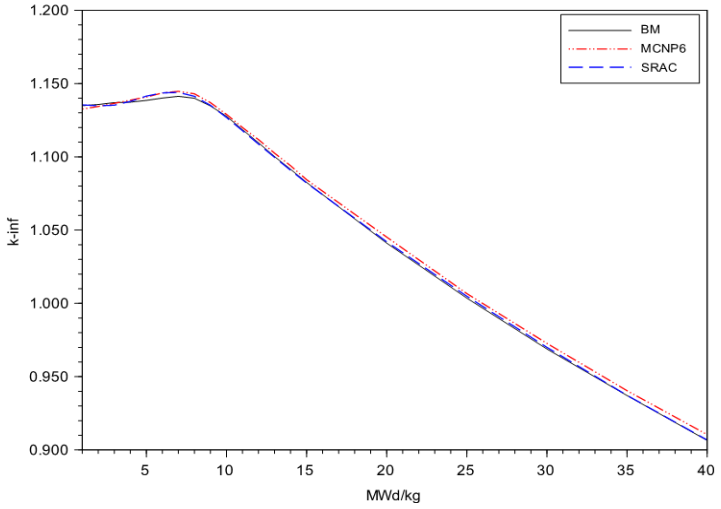

Fig. 3. Variation of k-inf of VVER-1000 LEU benchmark assembly versus burnup

As can be seen in Fig. 5, the burnable absorbers ^{155}Gd and ^{157}Gd deplete quickly at the beginning burnup steps and such quick depletion can be simulated by both MCNP6 and SRAC2006. In particular, ^{157}Gd depletes faster than ^{155}Gd because of its larger thermal neutron absorption cross section ($^{Gd\text{-}155}\sigma_a$ = 60,801 barn and $^{Gd\text{-}157}\sigma_a$ = 253,939 barn at E=0.0253 eV). The maximum deviations of the MCNP6 and SRAC2006 results with the BM values are -53.1% and 65.14% for ^{157}Gd at 7 MWd/kgHM, respectively. Those maximum deviations are 24.13%, 14.98%, 25.62%, 3.06% and 61.67% for MCU, TVS-M, WIMS8A, HELIOS and MULTICELL, respectively. The discrepancies of ^{157}Gd was large at the first burnup values, because ^{157}Gd burns out quickly in the first burnup steps and its concentration becomes very small, leading to a large uncertainty in the calculation results.

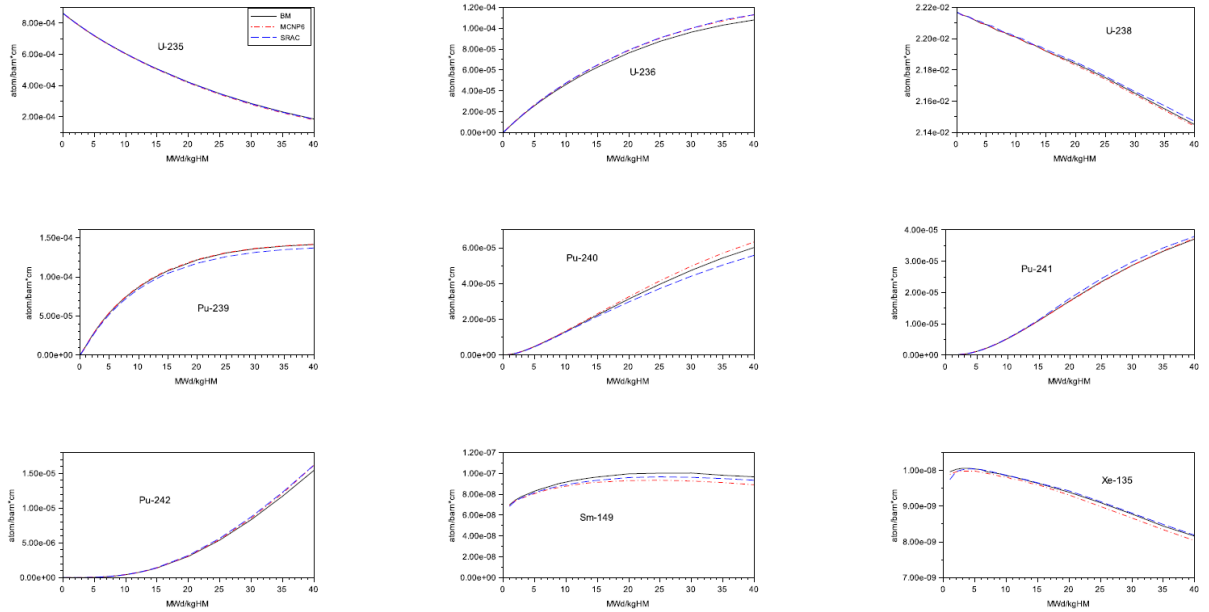

Fig. 4. Concentration of isotopes in Cell 1 as a function of burnup

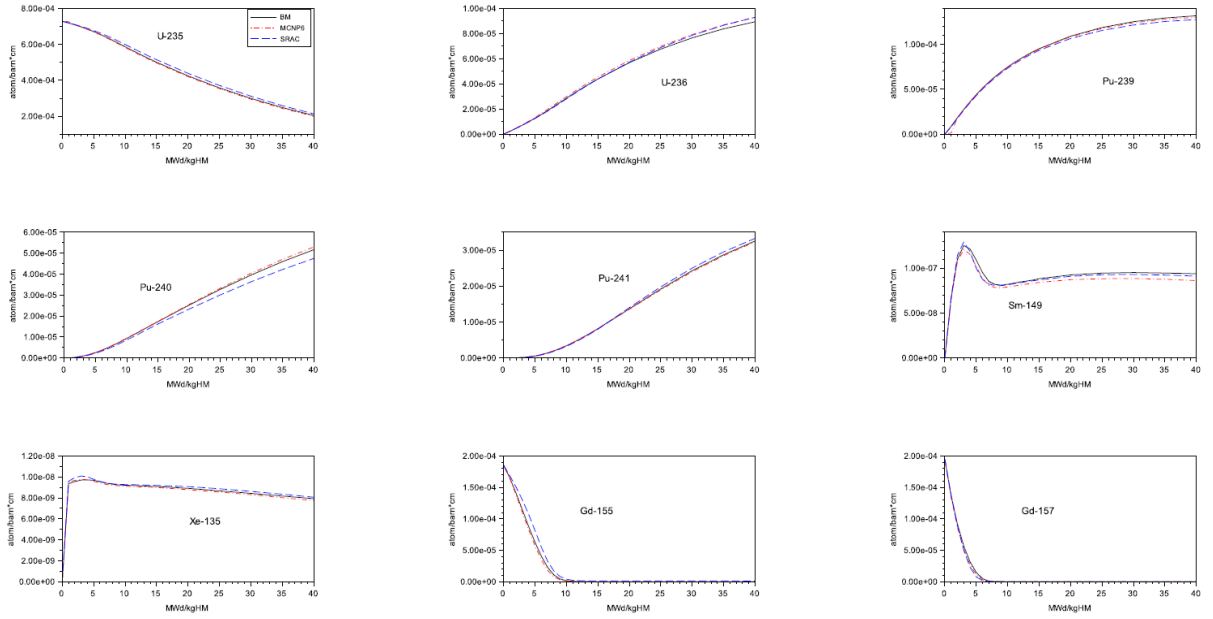

Fig. 5. Concentration of isotopes in Cell 24 as a function of burnup

C. Radial isotopic concentration in UGD rod

To investigate the variation of the isotopic composition in the radial direction of the UGD rod, Cell 24 was divided in to 5 regions to account for the shielding effect due to the gadolinium isotopes. The concentrations of ^{235}U, ^{239}Pu at 40 MWd/kgHM and ^{155}Gd và ^{157}Gd at 2 MWd/kgHM were calculated using MCNP6 and SRAC2006 and compared with the BM values as shown in Table II. It can be seen that the ^{235}U, ^{239}Pu, and ^{155}Gd concentrations versus radius calculated by MCNP6 were in good agreement with the BM values within 6.35%. However, the difference in the ^{157}Gd concentration calculated by MCNP6 and the BM values was as high as -32.45% at the outer zone. It is because that ^{157}Gd has very large thermal neutron absorption cross section as mentioned above and thus it burns most in the outer zone, where the thermal neutron flux is highest. Consequently, the concentration of ^{157}Gd at the outer zone is very small as compared to the inner zones, leading to a large statistical error.

The ^{235}U, ^{155}Gd and ^{157}Gd concentrations calculated by SRAC2006 generally agreed well with the BM values. However, the ^{239}Pu concentration calculated by SRAC2006 showed a big difference with the BM value for the radial fuel zone 4 of -24.36% as can be seen in Table II. The reason might be mainly due to the using of only four neutron energy groups for the lattice cell calculations with the PIJ module in which the spatial self-shielding effect of ^{238}U or any other resonant nuclide could not be properly taken into account.

Table II. Isotopic composition in Cell 24 vs radius, atoms/barn*cm

U-235 concentration vs radius in Cell 24 at 40 MWd/kgHM					
Fuel zone number	1	2	3	4	5
Radius, cm	0.173	0.244	0.299	0.345	0.386
BM	2.193E-04	2.126E-04	2.053E-04	1.975E-04	1.879E-04
MCNP6	2.135E-04	2.094E-04	1.998E-04	1.942E-04	1.818E-04
SRAC	2.277E-04	2.203E-04	2.116E-04	2.015E-04	1.889E-04
Discrepancy, % (MCNP6-BM)/BM	-2.64	-1.51	-2.68	-1.67	-3.25
Discrepancy, % (SRAC-BM)/BM	3.85	3.62	3.08	2.00	0.56
Pu-239 concentration vs radius in Cell 24 at 40 MWd/kgHM					
Fuel zone number	1	2	3	4	5
Radius, cm	0.173	0.244	0.299	0.345	0.386
BM	1.083E-04	1.107E-04	1.159E-04	1.273E-04	1.978E-04
MCNP6	1.065E-04	1.092E-04	1.139E-04	1.245E-04	1.967E-04
SRAC	9.847E-05	9.778E-05	9.699E-05	9.629E-05	2.083E-04
Discrepancy, % (MCNP6-BM)/BM	-1.66	-1.36	-1.73	-2.20	-0.56
Discrepancy, % (SRAC-BM)/BM	-9.07	-11.67	-16.31	-24.36	5.29
Gd-155 concentration vs radius in Cell 24 at 2 MWd/kgHM					
Fuel zone number	1	2	3	4	5
Radius, cm	0.173	0.244	0.299	0.345	0.386
BM	1.676E-04	1.636E-04	1.551E-04	1.333E-04	8.407E-05
MCNP6	1.676E-04	1.632E-04	1.530E-04	1.284E-04	7.873E-05
SRAC	1.704E-04	1.665E-04	1.580E-04	1.366E-04	8.536E-05
Discrepancy, % (MCNP6-BM)/BM	0.00	-0.24	-1.35	-3.68	-6.35
Discrepancy, % (SRAC-BM)/BM	1.67	1.80	1.86	2.44	1.54
Gd-157 concentration vs radius in Cell 24 at 2 MWd/kgHM					
Fuel zone number	1	2	3	4	5
Radius, cm	0.173	0.244	0.299	0.345	0.386
BM	1.502E-04	1.353E-04	1.074E-04	5.624E-05	8.722E-06
MCNP6	1.489E-04	1.328E-04	1.003E-04	4.674E-05	5.892E-06
SRAC	1.519E-04	1.373E-04	1.087E-04	5.716E-05	7.697E-06
Discrepancy, % (MCNP6-BM)/BM	-0.87	-1.85	-6.61	-16.89	-32.45
Discrepancy, % (SRAC-BM)/BM	1.15	1.51	1.20	1.64	-11.75

IV. CONCLUSIONS

A comparative burnup analysis of the OECD VVER-1000 LEU benchmark assembly was performed in this study using the Monte Carlo code MCNP6 and the deterministic code SRAC2006. The new depletion capability of MCNP6 and the OTF methodology for MCNP were applied in the the MCNP6 calculations; whereas the collision probability method based PIJ module of SRAC2006 was also utilized in this benchmarking calculation. The reactivity of the fuel assembly and the concentration of isotopes versus burnup obtained with MCNP6 and SRAC2006 generally show a good agreement with the BM values. The maximum difference in the k-inf calculated by MCNP6 and SRAC2006 with the BM values was 413 pcm and 352 pcm, respectively; while at the end of burnup (40 MWd/kgHM) the deviations in the nuclide concentrations calculated by MCNP6 and SRAC2006 with the BM values were generally within -7.93%. It was also found that the effect on the reactivity of the gadolinium burnable absorber and the depletion of the ^{155}Gd and ^{157}Gd isotopes at the beginning of the fuel cycle can be well simulated using MCNP6 and SRAC2006.

The isotopic composition variation of nuclides ^{235}U, ^{239}Pu, ^{155}Gd and ^{157}Gd as a function of radii of annular regions of the UGD rod was also calculated with MCNP6 and SRAC2006 and compared with the BM results. They were found to be generally in good agreement; however, the SRAC2006 results showed a large discrepancy with the BM values for the ^{239}Pu concentration that might be mainly due to the using of only four neutron energy groups in the SRAC2006 calculations. Consequently, it is highly recommended that MCNP6 and SRAC2006 can be used for burnup calculation of VVER-1000 fuel assemblies. Further investigation of the burnup calculation using MCNP6 and SRAC2006 at the full core level and MOX core of the VVER-1000 reactor is being planned.

REFERENCE

[1]. M. Kalugin, et al., A VVER-1000 LEU and MOX Assembly Computational Benchmark, Nuclear Energy Agency, NEA/NSC/DOC 10, 2002.

[2]. L. Thilagam, C. S. Sunny, V. Jagannathan, K. V. Subbaiah, “A VVER-1000 LEU and MOX assembly computational benchmark analysis using the lattice burnup code EXCEL”, Annals of Nuclear Energy 36, 505-519, 2009.

[3]. N. Petrov, G. Todorova, N. P. Kolev, “APOLLO2 and TRIPOLI4 solutions of the OECD VVER-1000 LEU and MOX assembly benchmark”, Annals of Nuclear Energy 55, 93–107, 2013.

[4]. M. Zheng, W. Tian, H. Wei, D. Zhang, Y. Wu, S. Qiu, G. Su, “Development of a MCNP–ORIGEN burn-up calculation code system and its accuracy assessment”, Annals of Nuclear Energy 63, 491–498, 2014.

[5]. L. Mercatali, A. Venturini, M. Daeubler, V. H. Sanchez, “SCALE and SERPENT solutions of the OECD VVER-1000 LEU and MOX burnup computational benchmark”, Annals of Nuclear Energy, 83, 328-341, 2015.

[6]. H. K. Louis, E. Amin, “The Effect of burnup on reactivity for VVER-1000 with MOXGD and UGD fuel assemblies using MCNPX code”, Journal of Nuclear and Particle Physics, 6 (3) 61-71, 2016.

[7]. S. A. Khan, V. Jagannathan, U. Kannan, A. Mathur, “Study of VVER-1000 OECD LEU and MOX computational benchmark with VISWAM code system”, Nuclear Energy and Technology 2, 312-334, 2016.

[8]. L. B. Vien, L. V. Vinh, H. T. Nghiem, N. K. Cuong, “Design analyses for full core conversion of the Dalat nuclear research reactor”, Nuclear Science and Technology, Vol. 4, No. 1, p.10-25, March 2014.

[9]. N. N. Dien, L. B. Vien, L. V. Vinh, H. T. Nghiem, N. K. Cuong, “Full core conversion and operational experience with LEU fuel of the Dalat nuclear research reactor”, RERTR 2014 - 35th International Meeting on Reduced Enrichment for Research and Test Reactors, IAEA Vienna Interational Center, Vienna, Austria, October 2014.

[10]. N. K. Cuong, H. T. Nghiem, V. H. Tan, “The Development of depletion program coupled with Monte Carlo computer code”, The 11th National Conference on Nuclear Science and Technology, Da Nang,Vietnam, August 2015.

[11]. N. H. Hiep, N. H. Tiep, T. V. Phu, N. T. Khai, “Development of an MCNP5-ORIGEN2 coupling scheme for burnup calculation of VVER-1000 fuel assemblies”, Nuclear Science and Technology, Vol. 6, No. 3, pp. 16-30, 2016.

[12]. D. B. Pelowitz et al., MCNP6TM User’s Manual, Version 1.0, LA-CP-13-00634, Rev. 0, 2013.

[13]. K. Okumura, T. Kugo, K. Kaneko, and K. Tsuchihashi, SRAC2006: A Comprehensive Neutronics Calculation Code System, JAEA-Data/Code 2007-004, 2007.

[14]. F. Brown, W. Martin, G. Yesilyurt, S. Wilderman, On-The-Fly Neutron Doppler Broadening for MCNP, Los Alamos National Laboratory, LA-UR-12-00700, 2012.